

10/696,021

## Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:sssptal204bxsd

PASSWORD :

TERMINAL (ENTER 1, 2, 3, OR ?):2

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 20:14:35 ON 11 MAY 2004

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 20:14:42 ON 11 MAY 2004  
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 10 MAY 2004 HIGHEST RN 681120-30-9  
DICTIONARY FILE UPDATES: 10 MAY 2004 HIGHEST RN 681120-30-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> fil casreact	SINCE FILE ENTRY	TOTAL SESSION
COST IN U.S. DOLLARS		
FULL ESTIMATED COST	0.42	0.63

FILE 'CASREACT' ENTERED AT 20:14:47 ON 11 MAY 2004  
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FILE CONTENT:1840 - 9 May 2004 VOL 140 ISS 19

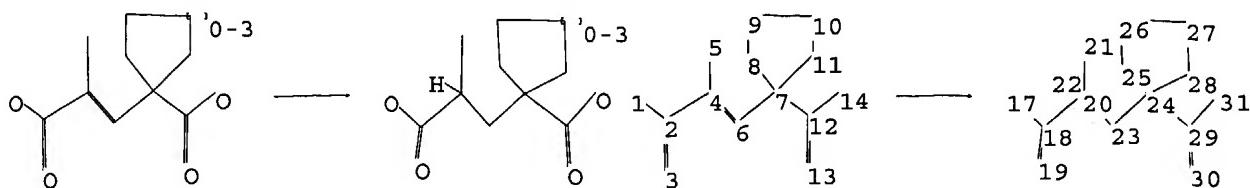
Some records from 1974 to 1991 are derived from the ZIC/VINITI data file and provided by InfoChem and some records are produced using some INPI data from the period prior to 1986.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Crossover limits have been increased. See HELP RNCROSSOVER for details.

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

=>  
Uploading C:\Program Files\Stnexp\Queries\10696021.str



chain nodes :

1 2 3 4 5 6 12 13 14 17 18 19 20 21 22 23 29 30 31

ring nodes :

7 8 9 10 11 24 25 26 27 28

chain bonds :

1-2 2-3 2-4 4-5 4-6 6-7 7-12 12-13 12-14 17-18 18-19 18-20 20-21 20-22  
20-23 23-24 24-29 29-30 29-31

ring bonds :

7-8 7-11 8-9 9-10 10-11 24-25 24-28 25-26 26-27 27-28

exact/norm bonds :

1-2 2-3 7-8 7-11 8-9 9-10 10-11 12-13 12-14 17-18 18-19 24-25 24-28  
25-26 26-27 27-28 29-30 29-31

exact bonds :

2-4 4-5 4-6 6-7 7-12 18-20 20-21 20-22 20-23 23-24 24-29

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom  
10:Atom 11:Atom 12:CLASS 13:CLASS 14:CLASS 17:CLASS 18:CLASS 19:CLASS  
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom  
29:CLASS 30:CLASS 31:CLASS

fragments assigned product role:

containing 17

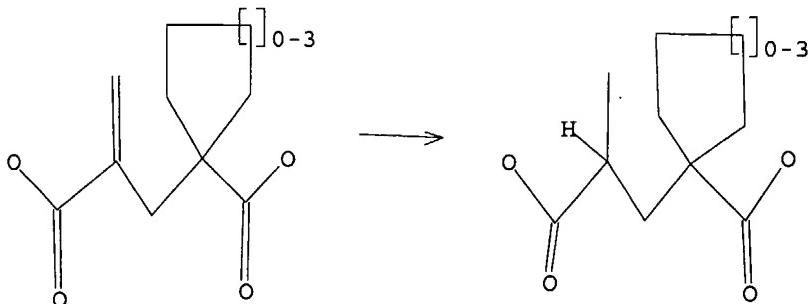
fragments assigned reactant/reagent role:

containing 1

L1 STRUCTURE UPLOADED

=> d query

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 20:15:11 FILE 'CASREACT'

SCREENING COMPLETE -

1 REACTIONS TO VERIFY FROM

1 DOCUMENTS

100.0% DONE 1 VERIFIED

0 HIT RXNS

0 DOCS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED VERIFICATIONS: 1 TO 79

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1 ( 0 REACTIONS)

=> s l1 full

FULL SEARCH INITIATED 20:15:15 FILE 'CASREACT'

SCREENING COMPLETE - 50 REACTIONS TO VERIFY FROM

14 DOCUMENTS

100.0% DONE 50 VERIFIED 0 HIT RXNS

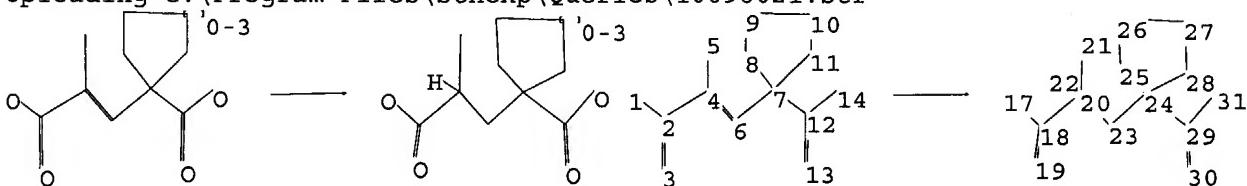
0 DOCS

SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1 ( 0 REACTIONS)

=>

Uploading C:\Program Files\Stnexp\Queries\10696021.str



chain nodes :

1 2 3 4 5 6 12 13 14 17 18 19 20 21 22 23 29 30 31

ring nodes :

7 8 9 10 11 24 25 26 27 28

chain bonds :

1-2 2-3 2-4 4-5 4-6 6-7 7-12 12-13 12-14 17-18 18-19 18-20 20-21 20-22  
20-23 23-24 24-29 29-30 29-31

ring bonds :

7-8 7-11 8-9 9-10 10-11 24-25 24-28 25-26 26-27 27-28

exact/norm bonds :

1-2 2-3 7-8 7-11 8-9 9-10 10-11 12-13 12-14 17-18 18-19 24-25 24-28  
25-26 26-27 27-28 29-30 29-31

exact bonds :

2-4 4-5 4-6 6-7 7-12 18-20 20-21 20-22 20-23 23-24 24-29

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:Atom 9:Atom  
10:Atom 11:Atom 12:CLASS 13:CLASS 14:CLASS 17:CLASS 18:CLASS 19:CLASS  
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom  
29:CLASS 30:CLASS 31:CLASS

fragments assigned product role:

containing 17

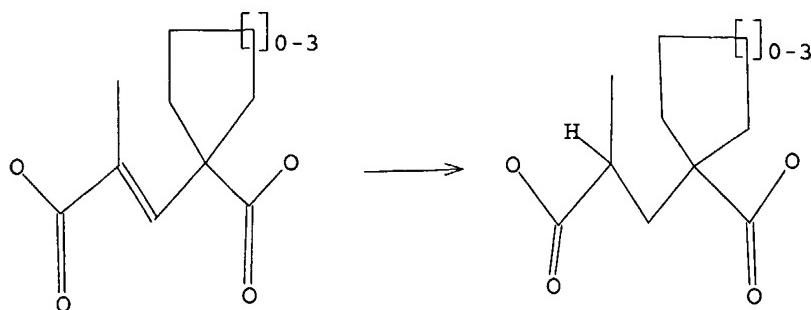
fragments assigned reactant/reagent role:

containing 1

L4 STRUCTURE UPLOADED

=> d query  
L4

STR



Structure attributes must be viewed using STN Express query preparation.

=> s 14

SAMPLE SEARCH INITIATED 20:16:24 FILE 'CASREACT'  
SCREENING COMPLETE - 1 REACTIONS TO VERIFY FROM 1 DOCUMENTS

100.0% DONE 1 VERIFIED 0 HIT RXNS 0 DOCS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED VERIFICATIONS: 1 TO 79

PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4 ( 0 REACTIONS)

=> s 14 full

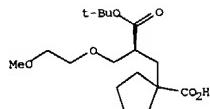
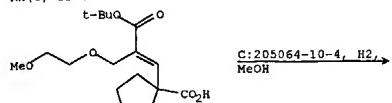
FULL SEARCH INITIATED 20:16:27 FILE 'CASREACT'  
SCREENING COMPLETE - 29 REACTIONS TO VERIFY FROM 10 DOCUMENTS

100.0% DONE 29 VERIFIED 8 HIT RXNS 3 DOCS  
SEARCH TIME: 00.00.01

L6 3 SEA SSS FUL L4 ( 8 REACTIONS)

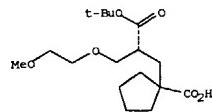
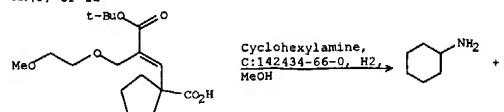
=> d 16 1-3

RX(6) OF 7



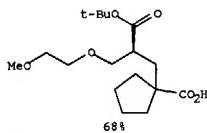
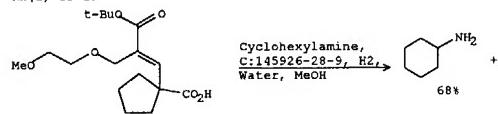
Na  
REF: Tetrahedron Letters, 42(42), 7481-7483; 2001  
NOTE: stereoselective, >97% ee, 26.degree., 5 bar H<sub>2</sub>

RX(5) OF 12



REF: Tetrahedron Letters, 40(11), 2187-2190; 1999  
NOTE: stereoselective, exampg. effect of chiral catalyst on asym. hydrogenation

RX(1) OF 19



REF: Eur. Pat. Appl., 644176, 22 Mar 1995  
NOTE: STEREOSELECTIVE, CHIRAL HYDROGENATION CATALYST

=> fil caplus		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	213.57	214.20

FILE 'CAPLUS' ENTERED AT 20:16:47 ON 11 MAY 2004  
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FILE COVERS 1907 - 11 May 2004 VOL 140 ISS 20  
FILE LAST UPDATED: 10 May 2004 (20040510/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s 16
L7          3 L6
=> d 17 1-3 abs ibib hitstr
```

L7 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN  
 AB The effectiveness of cyclooctadiene and norbornadiene precatalysts of the type [Rh(DuPHOS) (diolefin)]BF<sub>4</sub> in catalytic asym. hydrogenation of various prochiral olefins has been examined. In some of the systems studied, the NBD complex gave rise to the catalytically active species more rapidly than the corresponding COD complex, as expected. However, as catalyst loadings were reduced to levels more conducive to economic manufacture, the difference between the use of COD and NBD precatalysts became increasingly insignificant. This was conveniently highlighted by the formation of low enantiomeric excess products upon using an equimolar mixture of (S,S) and (R,R) precatalysts, bearing COD and NBD resp. With other substrates, the system displayed no induction time for either precatalyst and identical reaction profiles were observed.

ACCESSION NUMBER: 2001:708529 CAPLUS  
 DOCUMENT NUMBER: 136:150744  
 TITLE: On the economic application of DuPHOS rhodium(I) catalysts: a comparison of COD versus NBD precatalysts  
 AUTHOR(S): Cobley, C. J.; Lennon, I. C.; McCague, R.; Ramsden, J.  
 A.: Zanotti-Gerosa, A.  
 CORPORATE SOURCE: Chirotech Technology Ltd, Cambridge, CB4 0WG, UK  
 SOURCE: Tetrahedron Letters (2001), 42(42), 7481-7483 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 136:150744  
 REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN  
 AB A four step synthesis of a chiral glutarate half ester intermediate, required for the preparation of candoxatril, has been developed from t-Bu acrylate. The key steps in this route include a stereoselective synthesis of a trisubstituted alkene and its asym. hydrogenation with a Ru-BINAP catalyst.

ACCESSION NUMBER: 1999:180744 CAPLUS  
 DOCUMENT NUMBER: 130:296436  
 TITLE: Stereoselective synthesis of a candoxatril intermediate via asymmetric hydrogenation  
 AUTHOR(S): Challenger, Stephen; Derrick, Andrew; Mason, Clive P.; Silk, Terry V.  
 CORPORATE SOURCE: Pfizer  
 SOURCE: Central Research, Sandwich Kent, CT13 9NJ, UK  
 PUBLISHER: Tetrahedron Letters (1999), 40(11), 2187-2190  
 DOCUMENT TYPE: CODEN: TELEAY; ISSN: 0040-4039  
 LANGUAGE: Elsevier Science Ltd.  
 OTHER SOURCE(S): Journal  
 English  
 CASREACT 130:296436  
 REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN  
 GI For diagram(s), see printed CA Issue.  
 AB Title compds. (I, II; R = 5-indanyl, protecting group), are prepared by hydrogenating (E)-allylic ethers (III) or (IV) in the presence of a stereoselective Rh or Ru biphosphine catalyst and a protic solvent. Thus, III (R = Me<sub>3</sub>C) cyclohexylamine salt and [(R)-(+)-2,2'-bis(diphenylphosphino)-1,1'-binaphthyl]chloro(p-cymene)ruthenium chloride in H<sub>2</sub>O/MeOH were hydrogenated at 50 psi and 45-50° for 19 h to give 68% I (R = Me<sub>3</sub>C) cyclohexylamine salt (S:R = 99:1).

ACCESSION NUMBER: 1995:801435 CAPLUS  
 DOCUMENT NUMBER: 124:55417  
 TITLE: Asymmetric hydrogenation of (E)-1-[2-(tert-butoxycarbonyl)-3-(2-methoxyethoxy)prop-1-enyl]-1-cyclopentanecarboxylic acid and related compounds.  
 INVENTOR(S): Challenger, Stephen  
 PATENT ASSIGNEE(S): Pfizer Ltd., UK  
 SOURCE: Eur. Pat. Appl., 15 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 644176	A1	19950322	EP 1993-307517	19930922
EP 644176	B1	19951115		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
AT 130292	E	19951215	AT 1993-307517	19930922
ES 2041183	T3	19960216	ES 1993-307517	19930922
CA 2172374	AA	19950330	CA 1994-2172374	19940909
CA 2172374	C	19980526		
WO 9508526	A1	19950330	WO 1994-EP3036	19940909
W: AU, BR, CA, CN, CZ, FI, HU, JP, KR, NO, NZ, PL, RU, US				
AU 9477812	A1	19950410	AU 1994-77812	19940909
AU 679787	B2	19970710		
CN 1131940	A	19960925	CN 1994-193488	19940909
JP 08509988	T2	19961022	JP 1994-509535	19940909
JP 2771038	B2	19980702		
HU 74101	A2	19961128	HU 1996-716	19940909
BR 9407598	A	19970107	BR 1994-7598	19940909
RU 2114103	C1	19980627	RU 1996-107758	19940909
ZA 9407330	A	19960322	ZA 1994-7330	19940921
US 5618970	A	19970408	US 1996-612940	19960307
FI 9601308	A	19960321	FI 1996-1308	19960321
NO 9601149	A	19960521	NO 1996-1149	19960321
PRIORITY APPLN. INFO.:		EP 1993-307517	A	19930922
		WO 1994-EP3036	W	19940909
OTHER SOURCE(S):		CASREACT 124:55417; MARPAT 124:55417		

=> logoff Y		
COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	10.25	224.45
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.08	-2.08

STN INTERNATIONAL LOGOFF AT 20:20:16 ON 11 MAY 2004